# Bayes Coffee House: Probabilistic Bisimulation Metrics and Their Applications to Representation Learning

## Lecture 1: The logical characterization of bisimulation

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# Overview

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- Diffusion and continuous-time processes [MFPS 2019, 2020]

# Collaborators

Giorgio Bacci, Philippe Chaput, Linan Chen, Florence Clerc, Vincent Danos, Josée Desharnais, Abbas Edalat, Norm Ferns, Nathanaël Fijalkow, Robert Furber, Vineet Gupta, Radha Jagadeesan, Bartek Klin, Dexter Kozen, Kim Larsen, François Laviolette, Radu Mardare, Gordon Plotkin and Doina Precup.

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- a set of *labels* or *actions*, L or $\mathcal{A}$ and
- a transition relation $\subseteq S \times \mathcal{A} \times S$, usually written

$$\rightarrow_a \subseteq S \times S.$$

The transitions could be indeterminate (nondeterministic).

# Markov Chains

- A *discrete-time* Markov chain is a finite set $S$ (the state space) together with a transition probability function $T : S \times S \longrightarrow [0, 1]$.

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- A *discrete-time* Markov chain is a finite set $S$ (the state space) together with a transition probability function $T : S \times S \longrightarrow [0, 1]$.
- The key property is that the transition probability from $s$ to $s'$ only depends on $s$ and $s'$ and not on the past history of how it got there. This is what allows the probabilistic data to be given as a single matrix $T$.

# Discrete probabilistic transition systems

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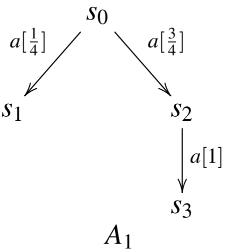
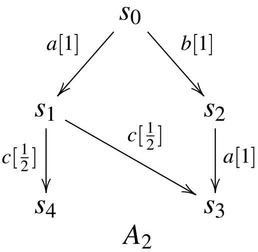
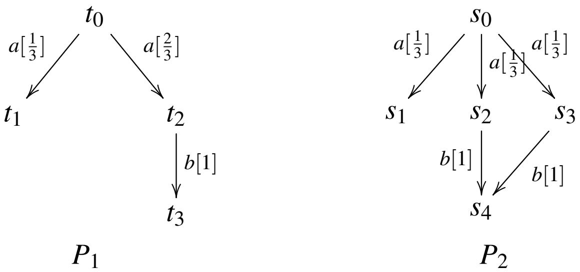
- $$(S, \mathsf{L}, \forall a \in \mathsf{L}\ T_a : S \times S \longrightarrow [0,1])$$
- The model is *reactive*: All probabilistic data is *internal* - no probabilities associated with environment behaviour.

# Examples of PTSs



- Consider


$t_0$
$a[\frac{1}{3}]$
$a[\frac{2}{3}]$
$t_1$
$t_2$
$b[1]$
$t_3$
$P_1$
$s_0$
$a[\frac{1}{3}]$
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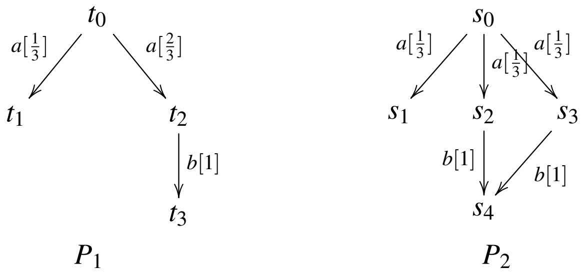
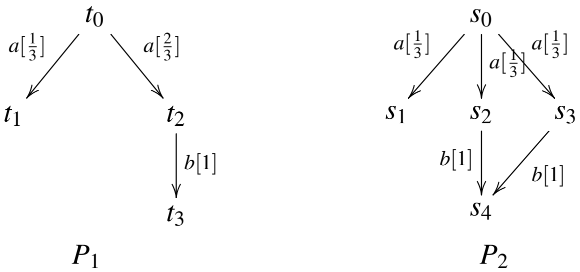



- Should $s_0$ and $t_0$ be bisimilar?

# Bisimulation for PTS: Larsen and Skou

- Consider




- Should $s_0$ and $t_0$ be bisimilar?
- Yes, but we need to add the probabilities.

# The Official Definition

- Let $\mathcal{S} = (S, \mathsf{L}, T_a)$ be a PTS. An equivalence relation $R$ on $S$ is a **bisimulation** if whenever $sRs'$, with $s, s' \in S$, we have that for all $a \in \mathcal{A}$ and every $R$-equivalence class, $A$, $T_a(s, A) = T_a(s', A)$.

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- The notation $T_a(s, A)$ means "the probability of starting from $s$ and jumping to a state in the set $A$."
- Two states are bisimilar if there is some bisimulation relation $R$ relating them.

# What are labelled Markov processes?

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- All probabilistic data is *internal* - no probabilities associated with environment behaviour.
- We observe the interactions - not the internal states.
- **In general, the state space of a labelled Markov process may be a *continuum*.**

# The Need for Measure Theory

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- Basic fact: There are subsets of $\mathbf{R}$ for which no sensible notion of size can be defined.
- More precisely, there is no non-trivial translation-invariant measure defined on all the subsets of the reals.

# Stochastic Kernels

- A *stochastic kernel* (Markov kernel) is a function $h : S \times \Sigma \longrightarrow [0, 1]$ with (a) $h(s, \cdot) : \Sigma \longrightarrow [0, 1]$ a (sub)probability measure and (b) $h(\cdot, A) : S \longrightarrow [0, 1]$ a measurable function.

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- and the uncountable generalization of a matrix.
- They are the Kleisli arrows of a monad: the Giry monad.

# Formal Definition of LMPs

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- $\forall s : S.\lambda A : \Sigma.\tau_\alpha(s, A)$ is a subprobability measure
  and
  $\forall A : \Sigma.\lambda s : S.\tau_\alpha(s, A)$ is a measurable function.

# Probabilistic Bisimulation

## Desharnais et al.

Let $\mathcal{S} = (S, i, \Sigma, \tau)$ be a labelled Markov process. An equivalence relation $R$ on $S$ is a **bisimulation** if whenever $sRs'$, with $s, s' \in S$, we have that for all $a \in \mathcal{A}$ and every $R$-closed measurable set $A \in \Sigma$, $\tau_a(s, A) = \tau_a(s', A)$.

Two states are bisimilar if they are related by a bisimulation relation.

# A game for bisimulation

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- A player loses when he or she cannot make a move. Note that if $C$ is all of the state space, duplicator loses. Duplicator wins if she can play forever.
- We prove that $x$ is bisimilar to $y$ iff Duplicator has a winning strategy starting from $(x, y)$.

# Logical Characterization

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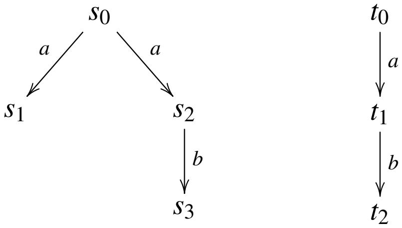
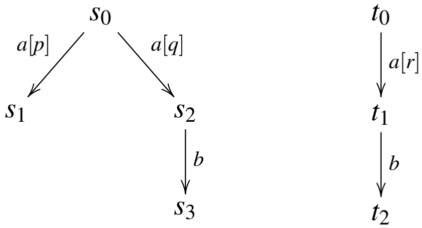
$$\exists A \in \Sigma.(\forall s' \in A. s' \models \phi) \wedge (\tau_a(s, A) > q).$$
- Two systems are bisimilar iff they obey the same formulas of $\mathcal{L}$. [DEP 1998 LICS, I and C 2002]

# That cannot be right?




Two processes that cannot be distinguished without negation.
The formula that distinguishes them is $\langle a \rangle (\neg \langle b \rangle \top)$.

# But it is!

- 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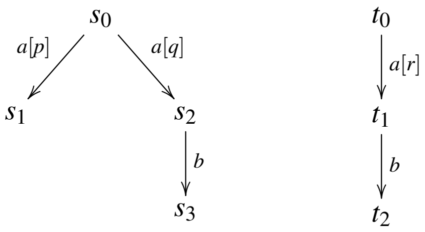
- 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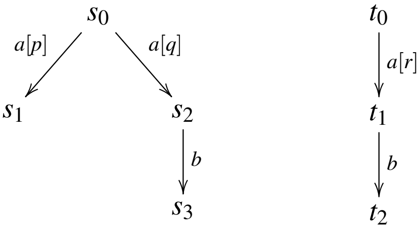
- 


  We add probabilities to the transitions.
- If $p + q < r$ or $p + q > r$ we can easily distinguish them.
- If $p + q = r$ and $p > 0$ then $q < r$ so $\langle a \rangle r \langle b \rangle 1 \top$ distinguishes them.

# Proof idea

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- Use Dynkin's lemma to show that we get a well defined measure on the $\sigma$-algebra generated by such sets and the above equality holds.
- Use special properties of analytic spaces to show that this $\sigma$-algebra is the same as the original $\sigma$-algebra.

# Simulation

Let $\mathcal{S} = (S, \Sigma, \tau)$ be a labelled Markov process. A preorder $R$ on $S$ is a **simulation** if whenever $sRs'$, we have that for all $a \in \mathcal{A}$ and every $R$-closed measurable set $A \in \Sigma$, $\tau_a(s, A) \leq \tau_a(s', A)$. We say $s$ is simulated by $s'$ if $sRs'$ for some simulation relation $R$.

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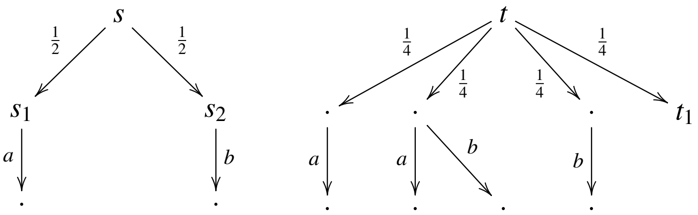
- One can show that if $s$ simulates $s'$ then $s$ satisfies all the formulas of $\mathcal{L}$ that $s'$ satisfies.
- What about the converse?

# Counter example!

In the following picture, $t$ satisfies all formulas of $\mathcal{L}$ that $s$ satisfies but $t$ does not simulate $s$.




All transitions from $s$ and $t$ are labelled by $a$.

# Counter example (contd.)

- A formula of $\mathcal{L}$ that is satisfied by $t$ but not by $s$.

$$\langle a\rangle_0(\langle a\rangle_0 \mathsf{T} \wedge \langle b\rangle_0 \mathsf{T}).$$

# Counter example (contd.)

- A formula of $\mathcal{L}$ that is satisfied by $t$ but not by $s$.

$$\langle a\rangle_0(\langle a\rangle_0 \mathsf{T} \wedge \langle b\rangle_0 \mathsf{T}).$$

- A formula with disjunction that is satisfied by $s$ but not by $t$:

$$\langle a\rangle_{\frac{3}{4}}(\langle a\rangle_0 \mathsf{T} \vee \langle b\rangle_0 \mathsf{T}).$$

# A logical characterization for simulation

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- The original proof uses domain theory and approximation.
- New development (2017 ICALP) we can prove logical characterization for simulation and bisimulation in almost the same way.

# Digression on Analytic Spaces

- An analytic set $A$ is the image of a Polish space $X$ (or a Borel subset of $X$) under a continuous (or measurable) function $f : X \to Y$, where $Y$ is Polish. If $(S, \Sigma)$ is a measurable space where $S$ is an analytic set in some ambient topological space and $\Sigma$ is the Borel $\sigma$-algebra on $S$.

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- Analytic sets do not form a $\sigma$-algebra but they are in the completion of the Borel algebra under **any** measure. [Universally measurable.]

# Amazing Facts about Analytic Spaces

- Given $A$ an analytic space and $\sim$ an equivalence relation such that there is a *countable* family of real-valued measurable functions $f_i : S \longrightarrow \mathbf{R}$ such that

$$\forall s, s' \in S. s \sim s' \iff \forall f_i. f_i(s) = f_i(s')$$

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  then the quotient space $(Q, \Omega)$ - where $Q = S/\sim$ and $\Omega$ is the finest $\sigma$-algebra making the canonical surjection $q : S \longrightarrow Q$ measurable - is also analytic.
- If an analytic space $(S, \Sigma)$ has a sub-$\sigma$-algebra $\Sigma_0$ of $\Sigma$ which separates points and is countably generated then $\Sigma_0$ is $\Sigma$! The Unique Structure Theorem (UST).

# Some more measure theory

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- $\lambda - \pi$ theorem: If $\Pi$ is a $\pi$-system and $\Lambda$ is a $\lambda$-system and $\Pi \subset \Lambda$ then $\sigma(\Pi) \subset \Lambda$.
- Corollary: If two measures agree on the sets of a $\pi$-system then they agree on the generated $\sigma$-algebra.

# Bisimulation proof I

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- We need to show there is a formula on which $x, y$ disagree.
- Let $\delta = \tau_a(x, \cdot)$ and $\gamma = \tau_a(y, \cdot)$.
- If $\delta(S) > \gamma(S)$ then choose *rational* $q$ such that $\delta(S) > q > \gamma(S)$. Now $x \models \langle a \rangle_q \top$ and $y \not\models \langle a \rangle_q \top$.

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- Duplicator chooses $x' \in C$ and $y' \notin C$ and claims that $x' \preceq y'$.
- $x \preceq y$ iff Duplicator has a winning strategy starting from $x, y$.

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- With these in place the proof of the logical characterization of simulation follows the same pattern.

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- However, if you require the transition functions to be continuous instead of measurable then logical characterization is restored.
- For simulation as well as bisimulation.
- We heavily use topological ideas in this proof.

# But...

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- We say “no”. A small change in the probability distributions may result in bisimilar processes no longer being bisimilar though they may be very “close” in behaviour.
- Instead one should have a (pseudo)metric for probabilistic processes.

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- Function $d : X \times X \longrightarrow \mathbb{R}^{\geq 0}$

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- If we insist on $d(x, y) = 0$ iff $x = y$ we get a *metric*.
- A pseudometric defines an equivalence relation: $x \sim y$ if $d(x, y) = 0$.
- Define $d^{\sim}$ on $X/\sim$ by $d^{\sim}([x], [y]) = d(x, y)$; well-defined by triangle. This is a proper metric.

# Bisimulation

- Let $R$ be an equivalence relation. $R$ is a bisimulation if: $s\ R\ t$ if $(\forall\ a)$:

$$(s \xrightarrow{a} P) \Rightarrow [t \xrightarrow{a} Q, P =_R Q]$$

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- $s, t$ are bisimilar if there is a bisimulation relating them.
- There is a maximum bisimulation relation.

# A putative definition of a metric-bisimulation

- $m$ is a metric-bisimulation if: $m(s,t) < \epsilon \Rightarrow$:

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- Problem: what is $m(P,Q)$? — Type mismatch!!
- Need a way to lift distances from states to a distances on distributions of states.

# A detour: Kantorovich metric

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- $$d(\mu, \nu) = \sup_f |\int f d\mu - \int f d\nu|, f \text{ 1-Lipschitz}$$
- Arises in the solution of an LP problem: *transshipment*.

# An LP version for Finite-State Spaces

When state space is finite: Let $P, Q$ be probability distributions. Then:

$$m(P,Q) = \max \sum_i (P(s_i) - Q(s_i))a_i$$

subject to:

$$\forall i. 0 \leq a_i \leq 1$$
$$\forall i,j.\ a_i - a_j \leq m(s_i, s_j).$$

# The dual form

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- $$\min \sum_{i,j} l_{ij} m(s_i, s_j) + \sum_i x_i + \sum_j y_j$$

  subject to:

  $$\begin{array}{l} \forall i.\ \sum_j l_{ij} + x_i = P(s_i) \\ \forall j.\ \sum_i l_{ij} + y_j = Q(s_j) \\ \forall i,j.\ l_{ij}, x_i, y_j \geq 0. \end{array}$$

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- We prove many equations by using the primal form to show one direction and the dual to show the other.

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  becomes $0$.
- This clearly cannot be lowered further so this is the min.

# Example 2

- Let $m(s,t) = r < 1$. Let $\delta_s$( resp. $\delta_t$) be the probability measure concentrated at $s$(resp. $t$). Then,

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$$\sum_{ij} l_{ij} m(s_i, s_j) = m(s,t) = r.$$

- Lower bound from primal: Choose $a_s = 0, a_t = r$, all others to match the constraints. Then

$$\sum_i (\delta_t(s_i) - \delta_s(s_i)) a_i = r.$$

# The Importance of Example 2

We can *isometrically* embed the original space in the metric space of distributions.

# Return from detour

## Summary

Given a metric on states in a metric space, can lift to a metric on probability distributions on states.

# Metric “bisimulation”

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- Thm: *Canonical least metric exists*.

# Tarski's theorem

If $L$ is a complete lattice and $F : L \longrightarrow L$ is monotone then the set of fixed points of $F$ with the induced order is itself a complete lattice. In particular there is a least fixed point and a greatest fixed point.

# Metrics: some details

- $\mathcal{M}$: $1$-bounded pseudometrics on states with ordering

$$m_1 \preceq m_2 \text{ if } (\forall s, t)\ [m_1(s,t) \geq m_2(s,t)]$$

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$$\begin{aligned}
\bot(s,t) &= \begin{cases} 0 \text{ if } s = t \\ 1 \text{ otherwise} \end{cases} \\
\top(s,t) &= 0, (\forall s, t) \\
(\sqcap\{m_i\}(s,t) &= \sup_i m_i(s,t)
\end{aligned}$$

# Greatest fixed-point definition

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- $F$ is monotone on $\mathcal{M}$, and metric-bisimulation is the greatest fixed point of $F$.
- The closure ordinal of F is $\omega$.

# Kantorovich-Rubinstein duality

## Definition

Given two probability measures $P_1, P_2$ on $(X, \Sigma)$, a *coupling* is a measure $Q$ on the product space $X \times X$ such that the marginals are $P_1, P_2$. Write $\mathcal{C}(P_1, P_2)$ for the set of couplings between $P_1, P_2$.

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## Theorem

Let $(X, d)$ be a compact metric space. Let $P_1, P_2$ be Borel probability measures on $X$

$$\sup_{f:X \longrightarrow [0,1] \text{ nonexpansive}} \left\{ \int_X f \mathrm{d}P_1 - \int_X f \mathrm{d}P_2 \right\} = \inf_{Q \in \mathcal{C}(P_1,P_2)} \left\{ \int_{X \times X} d \ \ \mathrm{d}Q \right\}$$